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PASSWORD:

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```
Web Page URLs for STN Seminar Schedule - N. America
NEWS
NEWS
                 "Ask CAS" for self-help around the clock
                 Powerful new interactive analysis and visualization software,
NEWS
         JUL 20
                 STN AnaVist, now available
NEWS
         AUG 11
                STN AnaVist workshops to be held in North America
NEWS 5
         AUG 30
                CA/CAplus -Increased access to 19th century research documents
NEWS 6 AUG 30
                CASREACT - Enhanced with displayable reaction conditions
NEWS 7 SEP 09
                ACD predicted properties enhanced in REGISTRY/ZREGISTRY
NEWS 8
        OCT 03
                MATHDI removed from STN
NEWS
         OCT 04
                CA/CAplus-Canadian Intellectual Property Office (CIPO) added
                 to core patent offices
        OCT 06
                 STN AnaVist workshops to be held in North America
NEWS 10
         OCT 13
                New CAS Information Use Policies Effective October 17, 2005
NEWS 11
NEWS 12
        OCT 17
                STN(R) AnaVist(TM), Version 1.01, allows the export/download
                 of CAplus documents for use in third-party analysis and
                 visualization tools
```

NEWS EXPRESS JUNE 13 CURRENT WINDOWS VERSION IS V8.0, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 13 JUNE 2005

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FILE 'HOME' ENTERED AT 08:45:31 ON 24 OCT 2005

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=> fil reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 08:46:05 ON 24 OCT 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 OCT 2005 HIGHEST RN 865836-54-0 DICTIONARY FILE UPDATES: 23 OCT 2005 HIGHEST RN 865836-54-0

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\QUERIES\10626356.str

O 1

chain nodes : 1 2 3 4 5 8 9 10 ring nodes:
15 16 17 18 19
chain bonds:
1-3 3-8 4-5 8-9 9-10
ring bonds:
15-16 15-19 16-17 17-18 18-19
exact/norm bonds:
1-3 3-8 4-5 8-9 9-10 15-16 15-19 16-17 17-18 18-19

G2:SO2,[*1]

Match level :

1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 8:CLASS 9:CLASS 10:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS

Generic attributes :

1:

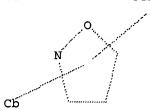
Number of Carbon Atoms : less than 7 Number of Hetero Atoms : less than 2 Type of Ring System : Monocyclic

Element Count :
Node 1: Limited
N,N1

O,00 S,S0 C,C4

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11 SAMPLE SEARCH INITIATED 08:46:40 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 9711 TO ITERATE

20.6% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

3 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 188315 TO 200125 PROJECTED ANSWERS: 63 TO 519

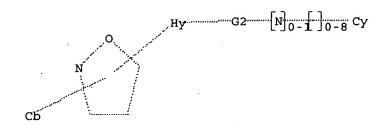
L2

3 SEA SSS SAM L1

```
FULL SEARCH INITIATED 08:46:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 192018 TO ITERATE
                                                              377 ANSWERS
100.0% PROCESSED
                 192018 ITERATIONS
SEARCH TIME: 00.00.02
            377 SEA SSS FUL L1
L3
=> s 13 and caplus/lc
      48312124 CAPLUS/LC
           368 L3 AND CAPLUS/LC
L4
=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\10626356.str
                   Hy G2 N0-10-8'y
                                                    16 <sub>21</sub>/18
                                                     15 19
0
:1
chain nodes :
1 2 3 4 5 8 9 10.
ring nodes :
15 16 17 18 19
chain bonds :
1-3 3-8 4-5 8-9 9-10
ring bonds :
15-16 15-19 16-17 17-18 18-19
exact/norm bonds :
1-3 3-8 4-5 8-9 9-10 15-16 15-19 16-17 17-18 18-19
G2:SO2,[*1]
Match level :
1:Atom 2:Atom 3:CLASS 4:CLASS 5:CLASS 8:CLASS 9:CLASS 10:Atom 15:Atom
16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:CLASS
Generic attributes :
1:
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : less than 2
Type of Ring System
                    : Monocyclic
Element Count :
Node 1: Limited
   N,N1
   0,00
   S,SO
   C, C4
```

=> s l1 full

=> d L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 subset=13 full FULL SUBSET SEARCH INITIATED 08:52:42 FILE 'REGISTRY' FULL SUBSET SCREEN SEARCH COMPLETED - 300 TO ITERATE

100.0% PROCESSED 300 ITERATIONS 173 ANSWERS SEARCH TIME: 00.00.01

L6 173 SEA SUB=L3 SSS FUL L5

=> s l6 and caplus/lc 48312124 CAPLUS/LC L7 173 L6 AND CAPLUS/LC

=> fil caplus
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
213.31 213.52

FILE 'CAPLUS' ENTERED AT 08:52:59 ON 24 OCT 2005
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http://www.cas.org/infopolicy.html

=> s 17

L8

3 L7

=> d ibib abs hitstr 1-3

L8 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 2005:158664 CAPLUS DOCUMENT NUMBER: 142:261539

DOCUMENT NUMBER: TITLE:

142:261539
Preparation of pyrrole-containing heterocyclic compounds as inhibitors of c-Met Aronov, Alex; Bandarage, Upul K.; Lauffer, David J. Vertex Pharmaceuticals Incorporated, USA; Li, Pan; Tomlinson, Ronald C. PCT Int. Appl., 61 pp. CODEN: PIXXD2

INVENTOR (S): PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE 20040816 WO 2005016920 20050224 WO 2004-US26749 A1 2005016920
W: AE, AG, AL,
CN, CO, CR,
GE, GH, GM,
LK, LR, LS,
NO, NZ, OM,
TJ, TM, TN,
RW: BW, GH, GM,
AZ, BY, KG,
EE, ES, FI,
SI, SK, TR,
SN, TD, TG
2005101650 A1 20050224 W0 2004-US26749
AM, AT. AU, AZ, BA, BB, BG, BR, BM, BY,
CU, C2, DE, DK, DM, D2, EC, EE, EG, ES,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,
LT, LU, LV, MA, MD, MG, HK, NN, MM, MX,
PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG,
KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY,
FR, GB, GR, HU, IE, IT, LU, MC, NL, PL,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ZM, CZ, PT, US 2005101650 Al 20050512 US 2004-919774 US 2003-495535P 20040816 P 20030815

PRIORITY APPLN. INFO.: OTHER SOURCE(S):

MARPAT 142:261539

The title compds. I [Q is an alkylidene chain wherein one methylene unit of Q is replaced by CO, O, etc.; R1 = H, optionally substituted ring, etc.; R2 = optionally substituted from the control of Q is replaced by CO, O, etc.; R1 = H, optionally substituted ring, etc.; R3 = CD, etc.] are nitrogens; n = 0 - 2: ring A = imidazole ring, etc.; R3 = CN, etc.] are prepared Thus, 4-[5-[2,3-difluorophenyl]isoxazol-4-yl]-lH-pyrcol-2-carboxylic acid (S-tetrahydrofuran-2-ylmethyl)amide was prepared in a multistep process from 1-(1-benzenesulfonyl-lH-pyrcol-3-yl)ethanone. In an in vitro test for the inhibition of c-Met kinase, compds. of this invention showed Ki values of 1 to > 10 µM.
845867-67-49 845867-55-59-845867-59-69
845867-61-OF 845867-62-1P 845867-59-19
RL: PAC (Pharmacological activity); STN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 845867-62-1 CAPLUS CN 1H-Fyrrole-2-carboxamide, 4-[3-(2,3-difluorophenyl)-4-isoxazolyl]-N-[3-(1H-imidazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

RN 845867-63-2 CAPLUS CN 1H-Pyrrole-2-carboxamide, N-(cyclopentylmethyl)-4-{3-(2,3-difluorophenyl)-4-isoxazolyl|- (9CI) (CA INDEX NAME) 845867-63-2 CAPLUS 1H-Pyrrole-2-carboxamide,

REFERENCE COUNT:

FORMAT

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

(Uses)
[prepn. of pyrrole-contg. heterocyclic compds. as inhibitors of c-Met)
845867-57-4 CAPLUS
Aretidine, 1-[[4-[5-(2,3-difluorophenyl]-4-isoxazolyl]-1H-pyrrol-2yl]carbonyl]- (9CI) (CA INDEX NAME)

845867-58-5 CAPLUS
1H-Pyrrole-2-carboxamide,
-(2,3-difluorophenyl)-4-isoxazolyl]-N-[3-(1H-imidazol-1-yl)propyl)- (9CI) (CA INDEX NAME) 845867-58-5

RN 845867-59-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide,
4-[5-{2,3-difluorophenyl}-4-isoxazolyl}-N-{[{2S}-tetrahydro-2-furanyl}methyl}- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

845867-61-0 CAPLUS Pyrrolidine, 1-[44-[3-(2,3-difluorophenyl)-4-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (SCI) (CA INDEX NAME)

L8 ANSWER 2 OF 3
ACCESSION NUMBER:
DOCUMENT NUMBER:
140:111220
TITLE:
Library
AUTHOR(S):
CORPORATE SOURCE:
CORPORATE SOURCE:
CORPORATE SOURCE:
CORPORATE SOURCE:
COPPORATE SOU Hwang, Sung Hee; Olmstead, Marilyn M.; Kurth, Mark J. Department of Chemistry, University of California, Davis, CA, 95616-5295, USA Journal of Combinatorial Chemistry (2004), 6(1), 142-148 CORPORATE SOURCE:

SOURCE:

CODEN: JCCHFF; ISSN: 1520-4766 American Chemical Society

PUBLISHER:

Journal English CASREACT 140:111220 DOCUMENT TYPE: LANGUAGE:

OTHER SOURCE (S):

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

A four-step solid-phase synthesis of isoxazolinopyrroles, e.g., I, that employs an acid-labile 2-(4-formyl-3-methoxyphenoxy)ethyl polystyrene HL resin is reported. Resin-bound vinyl sulfone II (Rl = PhCH2, 2-furanylmethyl, Me2CHCH2, MeOCH2CH2; X = resin) is obtained by DIC coupling of resin-bound amines with acid III (RZ = H, Me), which was in turn synthesized in solution phase by a regioselective nitrile oxide. 1,3-dipolar cycloaddn. The resin-bound pyrrole, e.g., IV, was hesized

hesized
on solid phase by pyrrole annulation with various isocyano derivs, and
potassium t-butoxide in which the sulfone q-anion generated by
Michael addition gives the desired pyrrole through internal condensation
followed by a sigmatropic [1,5]-hydrogen shift. The resulting
isoxazolinopyrrole; were released from resin by 10% TFA in moderate to
excellent to the sigmatropic [46064-13-3p
46064-14-19 64064-12-2P
46064-20-2P 64064-21-3P 64064-22-4P
46064-23-5P 64064-21-3P 64064-25-7P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP

(preparation of an isoxazolinopyrrole library via coupling of resin-bound

n-pound amines with sulfonylvinylisoxazolyl benzoic acids followed by pyrrole annulation with various isocyano derivs, and subsequent cleavage from the reasin) 646064-11-1 CAPLUS

NN 01000-1-1 CCO Senzamide, 4-(4,5-dihydro-5-methyl-5-[4-(phenylsulfonyl)-1H-pyrrol-3-yl]-3-isoxazolyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 646064-12-2 CAPLUS
CN Benzamide,
4-[4,5-dihydro-5-methyl-5-[4-(phenylsulfonyl)-1H-pyrrol-3-yl]-3isoxazolyl]-N-(2-furanylmethyl)- (9CI) (CA INDEX NAME)

RN 646064-13-3 CAPLUS
CN Benzamide,
4-[4,5-dihydro-5-methyl-5-[4-{phenylsulfonyl})-1H-pyrrol-3-yl}-3-isoxazolyl}-N-{2-methylpropyl}- (9CI) (CA INDEX NAME)

RN 646064-14-4 CAPLUS
CN Benzamide,
4-[4,5-dihydro-5-methyl-5-[4-[phenylsulfonyl]-1H-pyrrol-3-yl]-3isoxazolyl]-N-(2-methoxyethyl)- [9CI] (CA INDEX NAME)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

646064-21-3 CAPLUS
Benzamide, 4-{4,5-dihydro-5-methyl-5-{4-methyl-2-(1-piperidinylcarbonyl}-1H-pyrrol-3-yl}-3-isoxazolyl}-N-{2-methoxyethyl}- (9CI) (CA INDEX NAME)

646064-22-4 CAPLUS
Benzamide, 4-{4,5-dihydro-5-methyl-5-{4-methyl-2-{(4-methyl-1-1)-methyl)-1-1-pyrrol-3-yl}-3-isoxazolyl}-N-(phenylmethyl)-(9CI) (CA INDEX NAME)

646064-18-8 CAPLUS
Benzamide, 4-[4,5-dihydro-5-methyl-5-[4-methyl-2-(1-piperidinylcarbonyl)H-pyrrol-3-yll-3-isoxazolyl]-N-[phenylmethyl)- (9C1) (CA INDEX NAME)

646064-19-9 CAPLUS
Benzamide, 4-(4,5-dihydro-5-methyl-5-[4-methyl-2-(1-piperidinylcarbonyl)H-pyrrol-3-yl]-3-isoxazolyl]-N-(2-furanylmethyl)- (9C1) (CA IMDEX NAME)

646064-20-2 CAPLUS
Benzamide, 4-[4,5-dihydro-5-methyl-5-[4-methyl-2-(1-piperidinylcarbonyl)-1H-pyrrol-3-yl]-3-isoxazolyl]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

646064-23-5 CAPLUS
Benzamide, 4-[4,5-dihydro-5-methyl-5-[4-methyl-2-[(4-methylphenyl)sulfonyl]-lH-pyrrol-3-yl]-3-isoxazolyl]-N-(2-furanylmethyl)-(9CI) (CA INDEX NAME)

646064-24-6 CAPLUS
Benzamide, 4-[4,5-dihydro-5-methyl-5-[4-methyl-2-[(4-methyl)sulfonyl]-1H-pyrrol-3-yl]-3-isoxazolyl]-N-(2-methylpropyl)-(9CI) (CA INDEX NAME)

646064-25-7 CAPLUS
Benzamide, 4-[4,5-dihydro-5-methyl-5-[4-methyl-2-{{4-methyl-methyl-methyl-methyl-nl-methyl-nl-methyl-nl-methyl-nl-methoxyethyl-methyl-nl-methoxyethyl-methyl-methyl-methoxyethyl-meth

REFERENCE COUNT:

30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

(Continued)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN 404570-99-69 404571-00-2P 404571-01-3P 404571-02-4P 404571-03-5P 404571-07-9P 404571-07-9P 404571-07-9P 404571-07-9P 404571-07-9P 404571-07-9P 404571-13-7P 404571-13-5P 404571-13-5P 404571-13-7P 404571-13-9P 404571-13-9P 404571-13-9P 404571-13-9P 404571-13-9P 404571-13-9P 404571-13-9P 404571-25-P 404571-25-P 404571-27-3P 404571-27-3P 404571-27-3P 404571-27-3P 404571-31-9P 404571-31-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Uses)
(prepn. of isoxazolylpyrrole-2-carboxamides as ERK and AKT protein kinase inhibitors)
404570-75-8 CAPLUS
Morpholine, 4-[[4-[4-(2-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:220586 CAPLUS
DOCUMENT NUMBER: 136:247569
TITLE: Preparation of isoxazolylpyrrole-2-carboxamides as
ERK

and AKT protein kinase inhibitors Hale, Michael: Janetka, James: Haltais, Francois:

INVENTOR(S):

Jingrong: Mashal, Robert
Vertex Pharmaceuticals Incorporated, USA
PCT Int. Appl., 83 pp.
CODEN: PIXXD2
Patent
English 1

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

					KIND DATE												
								WO 2001-US28790									
	w:										, BG,						
											EE,						
											KG,						
											, HW,						
											TJ,						
											, KG,						
	RW:										TZ,						
											LU,						
											ML,						
											2001-						
ΑU	2001	0909	40		A5		2002	0326		AU 2	2001-	9094	D .		2	0010	914
US	2002	1776	18		Al		2002	1128		us a	2001-	9531	20		2	0010	914
US	6495	582			82		2002	1217			2001-						
EΡ	1317	453			A1		2003	0611		EP 2	2001-	9710	02		2	0010	914
	R:										IT,		LU,	NL,	SE,	MC,	PΤ,
		IE,	SI,	LT,	LV,	FI,	RO,	ΜK,	CY,	AL,	TR						
JΡ	2004	5091	19		T2		2004	0325		JP 2	2002-	5268	63		2	0010	914
ZΑ	2003	00169	96		A		2004	042B		ZA 2	2003-	1696			2	0010	914
NZ	5250	16			A		2004	1029		NZ 2	2001-	5250	16		2	0010	914
US	2003	1952	11		A1		2003	1016	1	US 2	2002~	2726	22		2	0021	015
US	2003 6649	640			B2		2003	1118									
NO	2003	00119	92		А		2003	0513	1	NO 2	2003-	1192			2	0030	314
US	2005	0905:	36		A1		2005	0428	1	US 2	2003-	6263	56		2	0030	724
ITY	APP	LN.	Info	:					1	US 2	2000-	2329	56P	- 1	P 2	00009	915

OTHER SOURCE(S): MARPAT 136:247569

WO 2001-US28790

W 20010914

R SOURCE(S): MARPAT 136:247569
Title compds., e.g., Ph2122CONNP2 (ZI = isoxazole-4,5-diyl, Z2 = pyrrole-4,2-diyl) were prepared Data for biol. activity of title compds. were given.

Were given.

404570-73-89 404570-76-99 404570-77-09
404570-78-19 404570-80-29
404570-78-19 404570-82-79 404570-80-59
404570-81-69 404570-85-09 404570-88-19
404570-91-29 404570-88-39 404570-89-49
404570-90-79 404570-91-69 404570-95-29
404570-90-39 404570-94-19 404570-95-29
404570-96-39 404570-97-49 404570-98-59

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404570-76-9 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(4-methoxyphenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404570-77-0 CAPLUS
1H-Pyrcole-2-carboxamide, 4-[4-(3-fluorophenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404570-78-1 CAPLUS 1H-Pyrrole-2-carbox

1H-Pyrrole-2-carboxamide, 4-[4-(3-methoxyphenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) 404570-79-2 CAPLUS 1H-Pyrrole-2-carboxamide, 4-[4-(2,5-dimethoxyphenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAWE)

404570-80-5 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3,4-difluorophenyl)-5-isoxazolyl]-N-[4pyridinylmathyl)- [9CI) (CA IMDEX NAME)

404570-81-6 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(2,3-difluorophenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404570-82-7 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(2,5-difluorophenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404570-86-1 CAPLUS
1H-Pyrrole-2-carboxamide, 4-(4-(3,4-difluorophenyl)-5-isoxazolyl)-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404570-87-2 CAPLUS
1H-Pyrrole-2-carboxamide, 4-(4-(2,3-difluorophenyl)-5-isoxazolyl)-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404570-88-3 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(2,5-difluorophenyl)-5-isoxazolyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN . (Continued)

404570-83-8 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(4-methoxyphenyl)-5-isoxazolyl)-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404570-84-9 CAPLUS
1H-Pyrrole-2-carboxamide, 4-{4-{3-fluorophenyl}-5-isoxazolyl}-N-{3-pyridinylmethyl}- {9CI} (CA INDEX NAME)

404570-85-0 CAPLUS 1H-Pyrrole-2-carboxamide, 4-[4-(3-methoxyphenyl)-5-isoxazolyl]-N-(3-pyridinylmethyl)- (9C1) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404570-89-4 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(4-methoxyphenyl)-5-isoxazolyl]-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

404570-90-7 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3-fluorophenyl)-5-isoxazolyl]-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

404570-91-8 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3-methoxyphenyl)-5-isoxarolyl]-N-[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

RN 404570-92-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-[3,4-difluorophenyl]-5-isoxazolyl]-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

(Continued)

- CH2-NH-C F
- RN 404570-93-0 CAPLUS
 CN H-Pytrole-2-carboxamide, 4-[4-[2,3-difluorophenyl)-5-isoxazolyl]-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)
- CH2-NH-C-NH-C-P
- RN 404570-94-1 CAPLUS CN 1H-Pyrcle-2-carboxamide, 4-[4-(2,5-difluorophenyl)-5-isoxazolyl]-N-[(cetrahydro-2-furanyl)methyl]- (9C1) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

- RN 404570-98-5 CAPLUS
 CN 1H-Pyrcole-2-carboxamide, N-[(1-ethyl-2-pyrrolidinyl)methyl]-4-[4-(3-methoxyphenyl)-5-isoxazolyl]- (9CI) (CA INDEX NAME)
- CH₂-NH-C
- RN 404570-99-6 CAPLUS
 CN 1H-Pyrrole-2-carboxamide, 4-[4-(2,5-dimethoxyphenyl)-5-isoxazolyl]-N-{{1-ethyl-2-pyrrolidinyl}methyl}- (9CI) (CA INDEX NAME)
- Et H CH2-NH-C- OME
- RN 404571-00-2 CAPLUS
 CN IH-Fyrrole-2-carboxamide, 4-[4-(3,4-difluorophenyl)-5-isoxazolyl]-N-[(1-ethyl-2-pyrrolidinyl)methyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continu

RN 404570-95-2 CAPLUS
CN IH-Pyrrole-2-carboxamide, N-[(1-ethyl-2-pyrrolidinyl)methyl]-4-[4-(4-fluorophenyl)-5-isoxarolyl]- (9C1) (CA INDEX NAME)

RN 404570-96-3 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-{(1-ethyl-2-pyrrolidinyl)methyl}-4-{4-(4-methoxyphenyl)-5-isoxazolyl}- (9CI) (CA INDEX NAME)

RN 404570-97-4 CAPLUS CN 1H-Pyrrole-2-carboxamide, N-[(1-ethyl-2-pyrrolidinyl)methyl]-4-[4-(3-fluorphenyl]-5-isoxazolyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-01-3 CAPLUS
CN H-Pytrole-2-carboxamide, 4-[4-[2,3-difluorophenyl)-5-isoxazolyl]-N-[[1-ethyl-2-pytrolidinyl]methyl]- (SCI) (CA INDEX NAME)

RN 404571-02-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-{4-{2,5-difluorophenyl}-5-isoxazolyl}-N-{{1-ethyl-2-pyrrolidinyl}methyl}- (9CI) {CA INDEX NAME}

RN 404571-03-5 CAPLUS
CN Morpholine, 4-[{4-{4-(3-methoxyphenyl)-5-isoxazolyl}-1H-pyrrol-2-yl}carbonyl}- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-04-6 CAPLUS

KN Horpholine, 4-[(4-14-(2,5-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2yllcarbonyl)- (9C1) (CA INDEX NAME)

RN 404571-05-7 CAPLUS CN Morpholine, 4-[[4-[4-[2,3-difluorophenyl]-5-isoxazolyl]-lH-pyrrol-2yl]carbonyl]- (9C1) (CA INDEX NAME)

RN 404571-06-8 CAPLUS
CN Morpholine, 4-[[4-[4-(2,5-difluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl- (9C1) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-11-5 CAPLUS
CN Piperazine, 1-[[4-[4-(2,5-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-12-6 CAPLUS
CN Piperazine, 1-{{4-{4-{2,3-difluorophenyl}}-5-isoxazolyl}-1H-pyrrol-2-yl}carbonyl}-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-13-7 CAPLUS
CN Piperazine, 1-[[4-[4-(2,5-difluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl)-4-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
RN 404571-07-9 CAPLUS
CN Piperazine, 1-[[4-[4-(4-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-08-0 CAPLUS
CN Piperazine, 1-{{4-{4-methoxyphenyl}-5-isoxazolyl}-1H-pyrrol-2yl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-09-1 CAPLUS
CN Piperazine, 1-[[4-[4-(3-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-10-4 CAPLUS
CN Piperazine, 1-[[4-[4-(3-methoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2yl[carbonyl]-4-methyl- (SCI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-14-8 CAPLUS CN 1H-Pyrrole-2-carboxamide, 4-[4-(3-chlorophenyl)-5-isoxazolyl]-N-(4pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 404571-15-9 CAPLUS
CN lh-Pyrrole-2-carboxemide, 4-[4-(3-chlorophenyl)-5-isoxazolyl)-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 404571-16-0 CAPLUS
CN lH-Pyrrole-2-carboxamide, 4-[4-[3-chlorophenyl)-5-isoxazolyl}-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

RN 404571-17-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide,
4-[4-(3-chlorophenyl)-5-isoxazoly])-N-[(1-ethyl-2-pyrrolidinyl)methyl}- (9CI) (CA INDEX NAME)

RN 404571-18-2 CAPLUS CN Piperazine, 1-[[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2yl[carbonyl]-4-methyl- (9CI) (CA IMDEX NAME)

RN 404571-19-3 CAPLUS
CN IN-Pyrrole-2-carboxamide, 4-[4-(4-chlorophenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (CO

RN 404571-23-9 CAPLUS
CN Morpholine, 4-[[4-{4-(4-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9C1) (CA INDEX NAME)

RN 404571-24-0 CAPLUS

Riperazine, 1-[|4-(4-(4-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2yllcarbonyll-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-25-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-[3,4-dichlorophenyl]-5-isoxazolyl]-N-[3-pyridinylmethyl)-[9CI] (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-20-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-(4-chlorophenyl)-5-isoxazolyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 404571-21-7 CAPLUS CN 1H-Pyrrole-2-carboxamide, 4-[4-(4-chlorophenyl)-5-isoxazolyl]-N-[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

RN 404571-22-8 CAPLUS CN 1H-Pyrrole-2-carboxamide, 4-{4-(4-cholorphenyl)-5-isoxazolyl}-N-[(1-ethyl-2-pyrrolidinyl)methyl}- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

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RN 404571-26-2 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-[3,4-dichlorophenyl]-5-isoxazolyl]-N-[(1-ethyl-2-pyrrolidinyl)methyl]- (9CI) (CA INDEX NAME)

RN 404571-27-3 CAPLUS
CN Morpholine, 4-[[4-[4-(3,4-dichlorophenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]- [9CI) (CA INDEX NAME)

RN 404571-28-4 CAPLUS CN Piperazine, 1-[[4-[4,4-dichlorophenyl]-5-isoxazolyl]-1H-pyrrol-2yl[carbonyl]-4-methyl- (9CI) (CA INDEX NAME) RN 404571-29-5 CAPLUS
CN 1H-Pyrclote2-cerboxamide, 4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-N(4-pyrldinylmethyl)- (9Cl) (CA INDEX NAME)

RN 404571-30-8 CAPLUS
CN HH-Pyrrole-2-carboxamide, 4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl}-N(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

RN 404571-31-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-N-

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 404571-35-3 CAPLUS
CN H-Pyrrole-2-carboxamide, 4-[4-(3-chloro-4-fluorophenyl)-5-isoxazolyl]-N(4-pyridinylmethyl)- (9C1) (CA INDEX NAME)

RN 404571-36-4 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-(3-chloro-4-fluorophenyl)-5-isoxazolyl]-N(3-pyridinylmethyl)- (9C1) (CA INDEX NAME)

RN 404571-37-5 CAPLUS
CN lH-Pyrrole2-carboxamide, 4-[4-(3-chloro-4-fluorophenyl)-5-isoxazolyl]-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) [(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

RN 404571-32-0 CAPLUS
CN IH-Pyrrole-2-carboxamide, 4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-N[(1-ethyl-2-pyrrolidinyl)mmethyl]- (9C1) (CA INDEX NAME)

RN 404571-33-1 CAPLUS
CN Morpholine, 4-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]- (SCI) (CA INDEX NAME)

RN 404571-34-2 CAPLUS
CN Plperazine, 1-[(4-(4-(3-chloro-2-fluorophenyl)-5-isoxazolyl)-1H-pyrrol-2-yllozhonyl)-4-methyl- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 404571-38-6 CAPLUS
CN H-Pyrrole2-carboxamide, 4-[4-(3-chloro-4-fluorophenyl)-5-isoxazolyl]-N[(1-ethyl-2-pyrrolidinyl)methyl]- (9C1) (CA INDEX NAME)

RN 404571-39-7 CAPLUS

Norpholine, 4-[[4-[4-(3-chloro-4-fluorophenyl]-5-isoxazolyl]-1H-pyrrol-2yllcarbonyl]- (9c1) (CA INDEX NAME)

RN 404571-40-0 CAPLUS
CN Piperazine, 1-[[4-[4-(3-chloro-4-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

404571-41-1 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404571-42-2 CAPLUS
IH-Pyrrole-2-carboxamide, 4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404571-43-3 CAPLUS IM-Pyrole-2-cacboxamide, 4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N-[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404571-54-6 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3,5-dichlorophenyl)-5-isoxazolyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

404571-55-7 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3,5-dichlorophenyl)-5-isoxazolyl]-N[(tetrahydro-2-furanyl)methyl]- (9CI) (CA INDEX NAME)

L8. ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

404571-44-4 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-{3,4-dimethoxyphenyl}-5-isoxazolyl}-N-{{1-ethyl-2-pyrrolidinyl}methyl]- (9CI) (CA INDEX NAME)

404571-45-5 CAPLUS Morpholine, 4-[[4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl]- (9CI) (CA INDEX NAME)

404571-46-6 CAPLUS
Piperazine, 1-{[4-(4-(3,4-dimethoxyphenyl)-5-isoxazolyl}-1H-pyrrol-2-yl]carbonyl|-4-methyl- (9CI) (CA INDEX NAME)

404571-53-5 CAPLUS
1H-Pyrrole-2-carboxamide, 4-[4-(3,5-dichlorophenyl)-5-isoxazolyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404571-56-8 CAPLUS
IM-Pyrrole-2-carboxamide, 4-(4-(3,5-dichlorophenyl)-5-isoxazolyl]-N-{(1-ethyl-2-pyrrolidinyl)methyl)- (9CI) (CA INDEX NAME)

404571-57-9 CAPLUS Morpholine, 4-[4-[4-(4-(3,5-dichlorophenyl)-5-isoxazolyl]-lH-pyrrol-2-yllcarbonyl]- (9C1) (CA INDEX NAME)

404571-58-0 CAPLUS
Piperazine, 1-[{4-{4-(3,5-dichlorophenyl)-5-isoxazolyl}-1H-pyrrol-2-yl}carbonyl}-4-methyl- (9CI) (CA INDEX NAME)

RN 404571-59-1 CAPLUS
CN Morpholine, 4-[[4-[4-(aminosulfonyl)-3-chlorophenyl]-5-isoxazolyl]-lHpyrrol-2-yllcarbonyl]- (9C1) (CA IMDEX NAME)

RN 404571-60-4 CAPLUS

Morpholline, 4-[[4-[3-chlorophenyl]-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl]- (CA INDEX NAME)

RN 404571-61-5 CAPLUS
CN Piperazine, 1-(2-fluorophenyl)-4-[[4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-

LB ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-65-9 CAPLUS
CN Isoquinoline, 2-[{4-{4-{3-chlorophenyl}}-5-isoxazolyl}-1H-pyrrol-2yl)carbonyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

RN 404571-66-0 CAPLUS
CN Isoquinoline, 1,2,3,4-tetrahydro-2-[{4-[4-(3-methylphenyl)-5-isoxazolyl]1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404571-67-1 CAPLUS
CN lH-Pyrrole-2-carboxamide, 4-[4-(3-chlorophenyl)-5-isoxazolyl]-N-methyl-N(phenylmethyl)- (GCI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404571-62-6 CAPLUS
CN Piperazine, 1-phenyl-4-{{4-(4-phenyl-5-isoxazolył)-1H-pyrrol-2-yl]carbonyl}- (9CI) (CA INDEX NAME)

RN 404571-63-7 CAPLUS
CN Piperazine, 1-[{4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl}carbonyl}-4-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 404571-64-8 CAPLUS
CN Piperazine, 1-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-phenyl- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-68-2 CAPLUS
CN 1H-Pyrcle-2-carboxamide, 4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-N-methyl-N-(phenyl)methyl)- (9C1) (CA INDEX NAME)

RN 404571-69-3 CAPLUS
CN Piperazine, 1-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-phenyl- [9CI] (CA INDEX NAME)

RN 404571-70-6 CAPLUS
CN Piperazine, 1-acetyl-4-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404571-71-7 CAPLUS
CN Isoquinoline, 2-[{4-{4-{3,4-dimethoxyphenyl}}-5-isoxazolyl}-1H-pyrrol-2yl[carbonyl]-1,2,3,4-tetrahydro-(SCI) (CA INDEX NAME)

RN 404571-72-8 CAPLUS
CN 3-Piperidinol, 1-[(4-[4-[3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9C1) (CA INDEX NAME)

RN 404571-73-9 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-{4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N-methyl-N-{2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) yl]carbonyl]-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 404571-77-3 CAPLUS
CN 1-Piperazineethanol, 4-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl]- (9CI) (CA INDEX NAME)

RN 404571-78-4 CAPLUS

1,4'-Bipiperidine, 1'-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl|carbonyl]- (GA INDEX NAME)

RN 404571-79-5 CAPLUS
CN 2-Piperidineethanol, 1-[{4-{4-{3,4-dimethoxyphenyl})-5-isoxazolyl}-1H-pyrrol-2-yl}carbonyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued

RN 404571-74-0 CAPLUS
CN 3-Piperidinol, 1-[{4-{4-(3-methylphenyl)-5-isoxazolyl}-1H-pyrrol-2-ylcarbonyl}- (SCI) (CA INDEX NAME)

RN 404571-75-1 CAPLUS
CN Piperazine, 1-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl)-4-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 404571-76-2 CAPLUS CN Piperazine, 1-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-80-8 CAPLUS
CN 2-Piperidineethanol, 1-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-lHpyrrol-2-yl|carbonyl]- [9CI) (CA INDEX NAME)

RN 404571-81-9 CAPLUS
CN Piperazine, 1-{(4-{4-(3-chloro-2-fluorophenyl)-5-isoxazolyl}-1H-pyrrol-2yl|carbonyl|-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 404571-82-0 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N[(1R,ZR)-2-hydroxy-1-methyl-2-phenylethyl)-N-methyl-, rel- (9CI) (CA
INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) Relative stereochemistry.

RN 404571-83-1 CAPLUS
CN Piperazine, 1-[(4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl]-4-(2-pyridinyl)- (9c1) (CA INDEX NAME)

RN 404571-84-2 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-(4-phenyl-5-isoxazolyl)-N-{2-(3-pyridinyl)ethyl}- (9CI) (CA INDEX NAME)

RN 404571-85-3 CAPLUS
CN Morpholine, 4-[(4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl]- (9CI)
(CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

RN 404571-89-7 CAPLUS
CN Pyrrolidine, 1-[[4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl[- (3CI) (CA INDEX NAME)

(Continued)

RN 404571-90-0 CAPLUS
CN Piperazine, 1-[[4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyll-4-phenyl- (9Cl) (CA INDEX NAME)

RN 404571-91-1 CAPLUS
CN Morpholine, 4-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2ylcarbonyl)- (9C1) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-86-4 CAPLUS CN Pyzrolidine, 1-{(4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl]-(9CI) (CA INDEX NAME)

RN 404571-87-5 CAPLUS
CN Pyridine, 4-(4-fluorophenyl)-1,2,3,6-tetrahydro-1-{[4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404571-88-6 CAPLUS
CN 1H-Pyrrole-2-carboxamide,
4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404571-92-2 CAPLUS
CN 1H-Pyrrole-2-carboxamide, 4-[4-(3-methylphenyl)-5-isoxazolyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 404571-93-3 CAPLUS
CN Pyrrolidine, 1-[[4-(4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404571-95-5 CAPLUS
CN Pyrrolidine,
1-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-, yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404571-96-6 CAPLUS
CN H-Pyrrole-2-carboxamide, 4-[4-(3-chlorophenyl)-5-isoxazolyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

404571-97-7 CAPLUS
Piperazine, 1-[{4-{4-(3-chlorophenyl)-5-isoxazolyl}-1H-pyrrol-2-yl]carbonyl}-4-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

(Continued)

404571-98-8 CAPLUS Pyrrolidine, 1-[(4-(4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl)- (9CI) (CA INDEX NAME)

RN 404571-99-9 CAPLUS
CN Pyridine,
1-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl}4-(4-fluorophenyl)-1,2,3,6-tetrahydro- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404572-03-8 CAPLUS 1H-Pyrrole-2-carboxamide, 4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-N-methyl-N-(phenylmethyl)- (SCI) (CA INDEX NAME)

404572-04-9 CAPLUS
Pyridine, 1-[[4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-(4-fluorophenyl)-1,2,3,6-tetrahydro- (9CI) (CA INDEX

404572-05-0 CAPLUS
Piperazine, 1-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-phenyl- (9CI) (CA INDEX NAME)

404572-00-5 CAPLUS
Piperazine, 1-[[4-[4-(3-chlorophenyl]-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-(2-pyridinyl)- (9CI) (CA INDEX NAME)

404572-01-6 CAPLUS 1H-Pyrrole-2-carboxamide, N-methyl-4-(4-phenyl-5-isoxazolyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

404572-02-7 CAPLUS
Piperazine,
4-methoxyphenyl)-4-[[4-(4-phenyl-5-isoxazolyl),1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404572-06-1 CAPLUS
1H-1,4-Diazejne, hexahydro-1-methyl-4-[[4-(4-(3-methylphenyl)-5isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

404572-07-2 CAPLUS
2-Piperidinemethanol, 1-[[4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl)carbonyl]- (9CI) (CA INDEX NAME)

RN 404572-08-3 CAPLUS
CN Isoquinoline,
1,2,3,4-tetrahydro-2-[[4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

404572-09-4 CAPLUS
Piperazine, 1-{[4-[4-[3,4-dimethoxyphenyl]-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]-4-[4-methoxyphenyl]- (9CI) (CA INDEX NAME)

404572-10-7 CAPLUS
Piperazine, 1-acetyl-4-[[4-[4-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1Hpyrrol-2-yllcarbonyl]- (9CI) (CA INDEX NAME)

404572-11-8 CAPLUS
1H-Pyrrole-2-carboxamide, N-methyl-4-[4-(3-methylphenyl)-5-isoxazolyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 404572-12-9 CAPLUS CN 2-Piperidinemethanol, 1-[{4-[4-[3-methylphenyl]-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9Cl) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (
RN 404572-16-3 CAPLUS
CN 1H-1,4-Diazepine,
1-[{4-14-(3,4-dimethoxyphenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]hexahydro-4-methyl- (9CI) (CA INDEX NAME) (Continued)

404572-17-4 CAPLUS
1H-1,4-Diazepine, 1-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl)hexahydro-4-methyl- (9CI) (CA INDEX NAME)

404572-18-5 CAPLUS
3-Piperidinol, 1-[{4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl](9CI) (CA INDEX NAME)

404572-20-9 CAPLUS
Piperazine, 1-acetyl-4-[[4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yllcarbonyl]- (9C1) (CA INDEX NAME)

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

RN 404572-13-0 CAPLUS
CN 2-Piperidinemethanol,
1-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2yl]carbonyl]- (9CI) (CA INDEX NAME)

404572-14-1 CAPLUS 2-Piperidineethanol, 1-[(4-(4-phenyl-5-isoxazolyl)-1H-pytrol-2-yllcarbonyl)- (9C1) (CA INDEX NAME)

404572-15-2 CAPLUS 2-Piperidineethanol, 1-{[4-(4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl)- (9C1) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404572-21-0 CAPLUS CN Piperazine, 1-(4-methoxyphenyl)-4-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

404572-22-1 CAPLUS
1-Piperazineethanol, 4-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl]- (9C1) (CA INDEX NAME)

404572-23-2 CAPLUS
1,4'-Bipiperidine, 1'-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyll- (9CI) (CA INDEX NAME)

(Continued)

RN 404572-24-3 CAPLUS
CN Pyridine,
4-(4-flucophenyl)-1,2,3,6-tetrahydro-1-[[4-{4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

404572-25-4 CAPLUS
Piperazine, l-acetyl-4-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

404572-26-5 CAPLUS IH-1,4-Diazepine, 1-[(4-(4-(3-chloro-2-fluorophenyi)-5-isoxazolyi]-1H-pyrroi-2-yl)carbonyl)hexahydro-4-methyl- (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

404572-31-2 CAPLUS
3-Piperidinol, 1-[[4-(4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyll- (9C1) (CA INDEX NAME)

404572-32-3 CAPLUS
Piperazine, 1-(4-(4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2yllcarbonyl]-4-(4-methoxyphenyl)- (SCI) (CA INDEX NAME)

404572-33-4 CAPLUS
1-Piperazineethanol, 4-[[4-[4-(3-chlorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl]- [9C1] (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

404572-28-7 CAPLUS
Piperazine, 1-acetyl-4-{{4-{4-(3-chloro-2-fluorophenyl)-5-isoxazolyl}-1Hpyrrol-2-yl|carbonyl|- (9C1) (CA INDEX NAME)

RN 404572-29-8 CAPLUS
CN Isoquinoline,
2-[[4-[4-[3-chloro-2-fluorophenyl]-5-isoxazolyl]-IH-pyrrol-2-yl]carbonyl]-1,2,3,4-tetrahydro- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

404572-35-6 'CAPLUS 1H-Pyrrole-2-carboxamide, 4-[4-(3-chlorophenyl)-5-isoxazolyl]-N-methyl-N-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

404572-36-7 CAPLUS
2-Piperidineethanol, 1-[[4-[4-(3-methylphenyl)-5-isoxazolyl]-1H-pyrrol-2-yllcarbonyl]- (9C1) (CA INDEX NAME)

 $\label{local-equation} $$404572-38-9$$ CAPLUS $$1H-Pyrrole-2-carboxamide, $4-[4-{3-chloro-2-fluorophenyl}-5-isoxazolyl]-N-[(1R,2R)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-, rel- (9CI) (CA INDEX NAME)$

Relative stereochemistry.

L8 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 404572-39-0 CAPLUS
CN 1,4'-Bipiperidine, 1'-[[4-[4-(3-chloro-2-fluorophenyl)-5-isoxazolyl]-1H-pyrrol-2-yl]carbonyl]- (9CI) (CA INDEX NAME)

RN 404572-40-3 CAPLUS
CN 4-Piperidinol, 1-[[4-(4-phenyl-5-isoxazolyl)-1H-pyrrol-2-yl]carbonyl](9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 18 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

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L1 STRUCTURE UPLOADED
L2 3 S L1
L3 377 S L1 FULL
L4 368 S L3 AND CAPLUS/LC
L5 STRUCTURE UPLOADED
L6 173 S L5 FULL SUB=L3
L7 173 S L6 AND CAPLUS/LC

FILE 'CAPLUS' ENTERED AT 08:52:59 ON 24 OCT 2005

FILE 'REGISTRY' ENTERED AT 08:53:22 ON 24 OCT 2005

=> s 14 not 17

L9 195 L4 NOT L7

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L10 60 L9

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             e.g., D SCAN or DISPLAY SCAN)
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             structure diagram, plus NTE and SEQ fields
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             its structure diagram
FHITSEQ ---- First HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
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=> d ibib abs hitstr 1-3

L10 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 2005:962251 CAPLUS DOCUMENT NUMBER: 143:266955

DOCUMENT NUMBER: TITLE:

143:266955

Synthesis of polyheterocyclic compounds as metabotropic glutamate receptor antagonists Arora, Jalaj: Edwards, Louise: Isaac, Methvin; Kers, Annika: Staaf, Karin: Slassi, Abdelmalik: Stefanac, Tomislav: Wensbo, David: Xin, Tao; Holm, Bjoern Astrazeneca AB, Swed: NPS Pharmaceuticals, Inc. PCT Int. Appl., 99 pp. CODEN: PIXXD2

Patent

English INVENTOR(S):

PATENT ASSIGNEE (S):

DOCUMENT TYPE: English

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PAT	PATENT NO.			KIND DATE				APPL	I CAT	DATE							
WO	2005080386			A1 2		20050901		WO 2005-US5216						20050217			
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GH,	HR,	ΗU,	ID,	IL,	IN,	ıs,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	sĸ,	SL,	SY,
		TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW
	RW:	BW,	GH,	GΜ,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	BJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	G₩,	ML,
		MR,	NE,	SN,	TD,	TG											
PRIORITY	RIORITY APPLN. INFO.:									US 2	004~	5452	92 P		P 2	0040	218

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L10 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

863647-39-6 CAPLUS
Pyridine, 3-[5-[2-[5-(3-chlorophenyl)-3-isoxazolyl]-1-pyrrolidinyl]-4-methyl-4H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

863647-40-9 CAPLUS
Pyridine, 4-[5-[2-[5-(3-chlorophenyl)-3-isoxazolyl]-1-pyrrolidinyl]-4cyclopropyl-4H-1,2,4-triazol-3-yl)- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN

The authors prepared polyheterocyclic compds. I [T = (hetero)aryl; W is attached to C atom on T. W = (Rl]m, Rl = OH, halo, NO2, OC1-C6-alkylhalo, C1-C6-alkyl, C2-C6-alkenyl, C1-C6-alkylhalo, C1-C6-alkyl(C0)RS, SO3RS, etc., RS = H, C1-C6-alkyl, C3-C7-cycloalkyl, aryl, m = 0-4; Y = (R3)p, Z

(R2]n, R2, R3 = OH, CO-C6-alkylcyano, O, NR5, NOR5, halo, OC1-C4-alkyl,
etc., n, p = 0-4; X1 = N, NR4, CR4, R4 = H, OH, C1-C6-alkyl,
CO-C6-alkylcyano, (SO)CO-C4-alkyl, (SO2)CO-C4-alkyl, etc.; X2 = C, N; X3

CR4, N, O; X4 = CR4, N, NR4, O; X5 = bond, CR4R8, NR4, O, S, SO, SOZ, R8 = undefined; X6 = CR4, N, X7 = C, N; Q = heterocycloalkyl, heteroaryll for use in treating mGluR5-mediated disorders such a neurol., psychiatric and gastrointestinal disorders as well as for treating chronic and acute pain disorders. Thus, 4-[(dimethylamino)ethoxy]benzolc acid hydrazide was reacted with piperidinecarboximidothioc acid Me ester II to give triazolylphenoxy di-He amine III.
853647-37-49 863647-43-95 863647-39-SP
863647-40-99 863647-41-09 863647-39-SP
863647-40-99 863647-41-09 863647-42-IP
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

IΤ

(preparation of polyheterocyclic compds., their metabotropic glutamate receptor antagonist activity, and use in treating mGluR5 mediated disorders) 863647-37-4 CAPLUS

NN 8038473-1 Cerum CM Morpholine, 4-[5-[5-[2-[5-[3-chlorophenyl)-3-isoxazolyl]-1-pyrrolidinyl]-4-cyclopropyl-44-1,2,4-triazol-3-yl]-2-pyridinyl]- (9CI) (CA INDEX NAME)

RN 863647-38-5 CAPLUS
CN Morpholine,
4-(5-[5-[2-[5-(3-chloropheny1)-3-isoxazoly1]-1-pyrrolidiny1]-4methyl-4H-1,2,4-triazol-3-y1}-2-pyridiny1]- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

863647-41-0 CAPLUS
Pyridine, 4-[5-[2-[5-(3-chlorophenyl)-3-isoxazolyl]-1-pyrrolidinyl]-4-methyl-4H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

863647-42-1 CAPLUS
Pyridine, 3-[5-[2-[5-(3-chlorophenyl)-3-isoxazolyl]-1-pyrrolidinyl]-4cyclopropyl-4H-1,2,4-triazol-3-yl]- (9CI) (CA INDEX NAME)

(Continued)

863647-31-8P 863647-32-9P 863647-33-0P
863647-34-1P 863647-35-2P 863647-36-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation of polyheterocyclic compds., their metabotropic glutamate receptor antagonist activity, and use in treating mGluR5 mediated disorders)
863647-31-8 CAPLUS
1-Pyrrolidinecarboxylic acid, 2-{5-(3-chlorophenyl)-3-isoxazolyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

863647-32-9 CAPLUS Isoxazole, 5-(3-chlorophenyl)-3-(2-pyrrolidinyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 863647-36-3 CAPLUS
CN 1-Pyrrolidinecarboximidothioic acid,
2-{5-(3-chorophenyl)-3-isoxazolyl}-Ncyclopropyl-, methyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

RN 863647-33-0 CAPLUS
CN 1-Pyrrolidinecarbothioamide,
2-[5-(3-chlorophenyl)-3-isoxazolyl]-N-methyl(9C1) (CA INDEX NAME)

863647-34-1 CAPLUS
1-Pyrrolidinecarbothioamide, 2-[5-(3-chlorophenyl)-3-isoxazolyl]-N-cyclopropyl- (9CI) (CA INDEX NAME)

863647-35-2 CAPLUS
1-Pyrrolidinecarboximidothioic acid,
-(3-chlorophenyl)-3-isoxazolyl]-Nmethyl-, methyl ester (9CI) (CA INDEX NAME)

L10 ANSWER 2 OF 60 CAPLUS COPYRIGHT 2005 ACS OR STN ACCESSION NUMBER: 2005:582509 CAPLUS DOCUMENT NUMBER: 143:115522 TITLE: A method 5

INVENTOR (5):

143:115522
A method for preparing 3,4-diphenyl-substituted isoxazole derivatives such as valdecoxib, parecoxib, and their intermediates Sundaram, Venketaraman: Bhimireddy, Anuradha; Eswaraiah, Sajja; Goverdhan, Gilla; Purandhar, Koilkonda; Rajendra, Surasani: Raju, Nadimpally Satyavarahala; Reddy, Anumula Raphupathi: Reddy, Lekkala Amarnath; Reddy, Enani Srinivasa; Reddy, Padi Prathap; Sampath, Alla; Sravanthi, Vecha Reddy: Laboratories Ltd., India; Reddy's Laboratories, Inc.
Eur. Pat. Appl., 15 pp.
CODEN: EPXXDW
Patent
English

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT N	٥.	KIND	DATE	APPLICATION N	O. DATE
EP 15506	58	A1	20050706	EP 2004-25818	1 20041230
R: 2	AT, BE, CH,	DE, I	DK, ES, FR,	GB, GR, IT, LI,	LU, NL, SE, MC, PT,
	IE, SI, LT,	LV,	FI, RO, MK,	CY, AL, TR, BG,	CZ, EE, HU, PL, SK,
1	BA, HR, IS,	YU			
US 20051	82113	A1	20050818	US 2004-25855	20041229
CA 24913	32	AA	20050630	CA 2004-24913	32 20041230
PRIORITY APPLI	N. INFO.:			IN 2003-CH106	3 A 20031230
				116 2004-50170	9B B 20040728

US 2004-637782P P 20041221

OTHER SOURCE(S): MARPAT 143:115522

AB The invention relates to a process for preparing 3,4-diphenyl-substituted isoxazole derivs. of formula I [wherein: X is H, SO2-alkyl, SO2NH2, or alkanoylamino-SO2] such as valdecoxib, parecoxib, and their intermediates.

intermediates.

For instance, 3,4-diphenyl-5-methylisoxazole (I, X is absent) was prepared
via one-pot cyclocondensation of benzonitrile oxide with
1-(1-methyl-2-phenylethenyl)pyrrolidine and subsequent pyrrolidine

removal

LIO ANSWER 2 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) of the obtained 3,4-diphenyl-5-methyl-5-pyrrolidinylisoxazoline with a yield of 22,24.

IT 857259-65-59

RE: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (method for preparing 3,4-diphenyl-substituted isoxazole derivs. such

85

RN CN

valdecoxib, parecoxib, and their intermediates)
857259-65-5 CAPLUS
180X8201e, 4,5-dihydro-5-methyl-3,4-diphenyl-5-(1-pyrrolidinyl)- (9CI)
(CA INDEX NAME)

REFERENCE COUNT: THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L10 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN

AB The title compds. I [R1 = CF3, alkyl, cycloalkyl, (cycloalkyl)alkyl; R2 = H, halo, CF3; R3 = H, OH, halo, etc.; NQ1 = N-linked saturated monocyclic 5-6 membered ring containing one N heteroatom and optionally comprising one

(Continued)

or more addnl. ring heteroatoms selected from N, O and S; Q2 = (un)substituted 5-6 membered heteroaryl comprising at least one ring heteroatom selected from N, O and S], useful in modulating insulin-like growth factor 1 receptor activity in a warm blooded animal such as man, were prepared Thus, reacting 2,5-dichloro-4-(5-methyl-lH-pyrazol-3-ylamino)pyrimidine with 2-[3-(pyridin-2-yl)isoxazol-5-yl)pyrrolidine (preparation given) in the presence EtN(iso-Pr)2 in n-hexanol afforded II. HCl.

The compds. I of the examples were found to have an IC50 of <100 µM in IGF-IR kinase assay. The pharmaceutical composition comprising the compound I is

compound I is

disclosed. 851432-02-5P 851432-03-6P 851432-09-2P 851432-10-5P 851433-96-0P

851432-10-5F 851433-96-UF RE: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES · (Uses)

(preparation of 4-(pyrazol-3-ylamino)pyrimidines for use in the treatment of

cancer)
831432-02-5 CAPLUS
4-Pyrimidinamine, 5-chloro-2-{2-(3-cyclopropyl-5-isoxazolyl)-1pyrrolidinyl}-N-(5-cyclopropyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 851432-03-6 CAPPLUS

CN 4-Pyrimidinamine, 5-chloro-2-[2-(3-cyclopropyl-5-isoxazolyl)-1pyrrolidinyl)-N-(5-methyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE RN 851432-09-2 CAPLUS

LIO ANSWER 3 OF 60
ACCESSION NUMBER:
DOCUMENT NUMBER:
1171LE:
INVENTOR(S):
PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE:

CAPLUS COPYRIGHT 2005 ACS on STN
2005:395305 CAPLUS
142:463737
Preparation of 4-(pyrazol-3-ylamino)pyrimidines for use in the treatment of cancer
Nowak, Thorsten; Thomas, Andrew Peter
Astrazeneca AB, Swed.; Astrazeneca UK Limited
PCT Int. Appl. 272 pp.
CODEM: PIXXD2

DOCUMENT TYPE:

DOCUMENT TYPE: English

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.			KIND DATE					APPL	I CAT	DATE							
							+										
WO 2005040159			Al 20050506				WO 2004-GB4307						20041011				
W:	AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
	CN,	co,	CR,	Cυ,	CZ,	DE,	DK,	DM,	DZ,	EC,	ĒE,	£G,	ES,	FI,	GB,	GD,	
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	
	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NΑ,	NI,	
	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	SY,	
	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	υz,	vc,	VN,	YU,	ZA,	ZM,	ZW	
RW:	BW,	GH,	GΜ,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
	AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
	EE,	ES,	FI,	FR,	GB,	GR,	ΗU,	ΙE,	IT,	ŁU,	MC,	NL,	PL,	PT,	RO,	SE,	
	SI.	SK.	TR.	BF.	BJ.	CF.	CG.	CI.	CH.	GA.	GN.	GO.	GW.	ML.	MR.	NE.	

SN, TD, TG PRIORITY APPLN. INFO.:

GB 2003-24335 A 20031017

GB 2004-12194

A 20040602

OTHER SOURCE(S):

MARPAT 142:463737

L10 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CN 4-Pyrimidinamine, 2-[2-(3-cyclopropyl-5-isoxazolyl)-1-pyrrolidinyl]-6(methoxymethyl)-N-(5-methyl-1H-pyrazol-3-yl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS, NOT DISPLAYED IN THE STRUCTURE
RN 851432-10-5 CAPIUS
CN 4-Pyrindinamine, 2-[2-(3-cyclopropyl-5-isoxazolyl)-1-pyrrolidinyl]-N-(5cyclopropyl-1H-pyrazol-3-yl)-6-(methoxymethyl)- (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 851433-96-0 CAPLUS
CN 4-Pyrimidinamine, .
2-{(ZS)-2-(3-cyclopropyl-5-isoxazolyl)-1-pyrrolidinyl]-N{5-cyclopropyl-1H-pyrazol-3-yl)-6-(methoxymethyl)- (9CI) {CA INDEX NAME}

Absolute stereochemistry.

one on more Tautomeric Double Bonds not Displayed in the Structure IT 851434-83-89, 2-(3-Cyclopropylisoxazol-5-y)lpytrolidine 851434-90-79 851434-91-8P, 2-[2-(3-Cyclopropylisoxazol-5-y)lpytrolidin-1-yl)-4-hydroxy-6-methoxymethylpytimidine

L10 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
851434-92-99, 4-Chloro-2-[2-(3-cyclopropylisoxazol-5-yl]pyrrolidin1-yl]-6-methoxymethylpyrimidine
RL: RCT (Reactant): SFN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of 4-(pyrazol-3-ylamino)pyrimidines for use in the treatment
of

of

cancer)
RN 851434-83-8 CAPLUS
CN . Isoxazole, 3-cyclopropyl-5-(2-pyrrolidinyl)- (9CI) (CA INDEX NAME)

851434-90-7 CAPLUS 1-Pyrrolidinecarboximidamide, 2-(3-cyclopropyl-5-isoxazolyl)-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 851434-89-4 CMF C11 H16 N4 O

. CM 2

CRN 7664-93-9 CMF H2 O4 S

851434-91-8 CAPLUS
4(1H)-Pyrimidinone, 2-{2-(3-cyclopropyl-5-isoxazolyl)-1-pyrrolidinyl}-6[methoxymethyl)- {9CI} (CA INDEX NAME)

L10 ANSWER 3 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN

851434-92-9 CAPLUS
Pyrimidine, 4-chloro-2-{2-(3-cyclopropyi-5-isoxazolyl)-1-pyrrolidinyl}-6(methoxymethyl)- (9CI) (CA INDEX NAME)

1

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

=> d ibib abs hitstr 57-60

L10 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1966:438483 CAPLUS
DOCUMENT NUMBER: 65:38483
ORIGINAL REFERENCE NO: 55:7160g-h,7161a-d
CONVENIENT SYNTHESIS OF INDOXAZENES
BIANCHI, Giorgio; Frati, Enzo
CORPORATE SOURCE: Univ. Pavia GAZZETTA Chimica Italiana (1966), 96(5), 559-65 CODEN: GCITA9; ISSN: 0016-5603 SOURCE : CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

IANGUAGE: Italian

GI For diagram(s), see printed CA Issue.

3 -Aryltetrahydroindoxazenes, obtained by the condensation of the appropriate nitrile oxides with suitable cyclohexanone enamines and subsequent treatment with acids, were dehydrogenated with N-bromosuccinimide to the corresponding 3-arylindoxazenes (I).

3-Phenylnaphtho[2,1-d]isoxazole (II) and the [1,2-d]-isomer were also prepared in this manner. a-Tetralone condensed with pyrrolidine yielded 181 1-pyrrolidino-3,4-dihydronaphthalene, b0.25, 102-4*.

m-OZNC6H4CN(O), m. 82-3*, was prepared from m-oZNC6H4C:NOH)OH with 1 mole equivalent NaOEt. The appropriate nitrile oxide and enamine (equimolar) m-O2NCGH4CN(O), m. 82-3*, was prepared from m-O2NCGH4C(:NOH)OR with 1 mole equivalent NaOEL. The appropriate nitrile oxide and enamine (equimolar amts.) in Et2O refluxed 2 hrs. yielded the corresponding IV (X = morpholino or pytrolidino) which were also obtained by adding dropwise with cooling the appropriate arylbenthydroxamyl chloride (V) in Et2O to equimolar amts. enamine and Et3N or by treating the V in Et2O with 1 equivalent enamine. The following compds. were prepared by these methods (m.p.,

Amax in mu, and log c given): IV (Ar = hh, R = H, X = morpholino), 91-2* (iso-Pr2O), 264, 4.10; IV (Ar = m-O2NC6H4, R = H, X = pyrrolidino), 96-7* (EtOH), 260, 4.26; IV (Ar = Ph, R = Me, X = pyrrolidino), 96-7* (EtOH), 260, 4.26; IV (Ar = Ph, R = Me, X = pyrrolidino) (VII), 148* (MeOH), 264, 4.16; VIII (X = morpholino) (IX), 241* (AcoEt or PhNO2), 256, 4.02. The appropriate IV and VII and IX refluxed 1-2 hrs. with 101 M2SO4 yielded 50-90% of the following compds. (same data given): IVa (Ar = m-O2NC6H4, R = H), 126* (EtOH), 230, 4.30; VIA (Ar = Ph, R = Me), 60* (MeOH), 240, 4.09; X, 120* (MeOH), 227 (2285, 300), 4.39 (4.22, 4.12); XI, 88* (MeOM), 257, 4.04. The appropriate IVa and X and XI (0.02 mole) in CC14 treated with 0.04, 0.02, and 0.02 mole equivs. N-bromosuccinimide and a trace (Me2C(CN)N:12, refluxed, treated with AcONa in the presence of AcOH or with KOH-MeOH yielded the following compds. (8 yield and m.p. given):

[Ar = Ph, R = H), 53, 82.5*; I (Ar = m-O2NC6H4, R = H) (XII), 90, or with KOH-MeOH yielded the following compds. (% yield and m.p. given):

[Ar = Ph, R = H), 53, 82.5°; I (Ar = m-o2NC6H4, R = H) (XII), 90, 171-2° (C6H6); I (Ar = Ph, R = Me), --, 92-3° (MeOH); II, 67, 133° (MeOH); III, 92, 62-3° (petroleum ether). In the preparation of XII, the intermediary yellow

3-(3-nitrophenyl)-4,7-dibromo4,5,6,7-tetrahydroindoxazene, m. 154-5°, could be isolated in 70% yield. III in 95% EtOH hydrogenated over Raney Ni, and the crude product heated 20 min. with 50% 182504 yielded 91% yellow 1-benzoyl-2-naphthol, m. 66° (petroleum ether).

IT 7007-73-0, Naphth(2,1-dijaoxazole, 3a,4,5,9b-tetrahydro-3-phenyl-9b-(1-pyrrolidinyl)-7007-74-1, 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-5-methyl-3-phenyl-1-a-(1-pyrrolidinyl)-7007-75-2, 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-3-(m-nitrophenyl)-7a-(1-pyrrolidinyl)-(preparation of)

N Naphth(2,1-di)isoxazole,
3a,4,5,9b-tetrahydro-3-phenyl-9b-(1-pyrrolidinyl)-

L10 ANSWER 58 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:418213 CAPLUS
OCCUMENT NUMBER: 61:18213
ORIGINAL REFERENCE NO.: 61:3089cTITLE: Enamines as 1,3-dipolarophiles
AUTHOR(\$): Kuchne, Martin E.; Weaver, J.; Franz, Peter
Univ. of Vermont, Burlington
Journal of Organic Chemistry (1964), 29(6), 1582-6
CODEN: JOCEAR; ISSN: 0022-3263
JOURNET TYPE: Journal of Organic Chemistry (1964), 29(6), 1582-6
CODEN: JOCEAR; ISSN: 0022-3263
JOURNEL SI: CASREACT 61:18213
GI For diagram(\$), see printed CA Issue.
AB The reactions of benzhydroxamoyl chloride and N1-a-chlorobenzylideneN2-phenylhydrazine with cyclic and acyclic enamines led to
aminodihydroisoxazoles e.g. I, and a pyrrolidinodihydropyrazole (II).
Elimination of the tertiary amine from the substituted heterocycles gave
the corresponding isoxazoles, e.g. III; tetrahydroisoindazoles, e.g. IV,
were obtained directly, except in the case of the reaction leading first
to II. Fyrazoles were also obtained.
IT 95867-86-2, 2-Isoxazoline, 3,4,5-triphenyl-5-(1-pyrrolidinyl)97847-70-6, 4H-Cyclopent(d]soxazole, 3a,5,6,6a-tetrahydro-3phenyl-6a-(1-pyrrolidinyl)(yreparation of)
RN 95867-96-2 CAPLUS
CN 2-Isoxazoline, 3,4,5-triphenyl-5-(1-pyrrolidinyl)- (7CI) (CA INDEX NAME)



97847-70-6 CAPLUS
4H-Cyclopent[d]isoxazole, 3a,5,6,6a-tetrahydro-3-phenyl-6a-(1-pyrrolidinyl)- (7CI, 9CI) (CA INDEX NAME)

98563-49-6 CAPLUS
4H-Cyclohept[d]isoxazole, 3a,5,6,7,8,8a-hexahydro-3-phenyl-8a-(1-pyrrolidinyl)- (7CI) (CA INDEX NAME)

L10 ANSWER 57 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (7CI, 8CI) (CA INDEX NAME) (Continued)

7007-74-1 CAPLUS 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-5-methyl-3-phenyl-7a-(1-pyrrolidinyl)- (7CI, BCI) (CA INDEX NAME)

7007-75-2 CAPLUS 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-3-(m-nitrophenyl)-7a-(1-pyrrolidinyl)- (7cI, 8cI) (CA INDEX NAME)

L10 ANSWER 58 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



L10 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1964:418212 CAPLUS

DOCUMENT NUMBER: ORIGINAL REFERENCE NO.:

AUTHOR (S):

CORPORATE SOURCE:

1964:418212 CAPIJUS
61:18212
61:3088e-N, 3099a-c
2,2'-Dicarbamoyl-5,5'-dinitrodiphenyl disulfides and
6-nitro-1,2-benzisothiazolones
Ponci, R.; Gialdi, F.; Baruffini, A.
Univ. Pavia, Italy
Farmaco, Edizione Scientifica (1964), 19(3), 254-68
CODEN: FRPSAX; ISSN: 0430-0920 SOURCE:

CODEN: FRPSAX; ISSN: 0430-0920

DOCUMENT TYPE:
JOURNAL DAGE:
Unavailable

CASRACT 61:18212

GI For diagram(s), see printed CA Issue.
A solution of 16 g. 2-thiorysnato-4-nitrobenzoic acid (prepared from 4-nitroanthranilic acid by the Sandmeyer reaction) in 300 ml. 201 KOH was kept on a water bath gradually heated during 30 min. to 90°, heated 30 min. at 90°, cooled, acidified with concentrated HCl, and chilled to precipitate yellow 2-mercapto-4-nitrobenzoic acid (I); 5-benzyl derivative, yellow,
m. 197-9° (dilute EtOH, C6H6). To the moist I dissolved in hot EtOH was added an equal volume cold EtOH and half volume 101 H2SO4, the mixture

interest of the standard o

treated dropwise with 5% iodine-EtOH to complete oxidation an equal me dilute

me dilute
HZSO4 added, and the whole chilled 24 hrs., filtered off, and the solid
washed with EtOH, Et2O, and petr. ether to give 701 2,2°-dicarboxy-5,5°dinitrodiphenyl disulfide (II), yellow, m. 280-2° (glacial AcOH).
To a suspension of 20 g. dry II in 140 ml. anhydrous C6H6, 25 g. PCIS was
added, the mixture refluxed 1 hr., decolorized with C, filtered, 4 vols.
petr. ether added, the mixture kept a long time at 0°, filtered off,
and the solid washed with petr. ether and crystallized from C6H6-petr.

ether to
yield 2,2'-dicarboxy-5,5'-dinitrodiphenyl disulfide dichloride (III),
yellow, m. 170-1'. III (2.16 g.).in min. cold dioxane was added
dropwise to a solution of 2 ml. concentrated NH3 in 13 ml. dioxane, the
mixture kept
15 min. at room temperature, 3 vols. H2O added, the mixture neutralized
with AcOH,
and the precipitate filtered off, and washed with H2O, then EtOH and
Et2O to

to yield 2,2'-dicarbamoyl-5,5'-dinitrodiphenyl disulfide (IV), yellow, m. 265-6' (AcOH). III analogously treated with BuNH2 and PhNH2 yielded, resp., 2,2'-bis(N-butylcarbamoyl)-5,5'-dinitrodiphenyl disulfide (V) pale yellow, m. 227-9' (AcOH), and 2,2'-dicarbanilino-5,5'-dinitrodiphenyl disulfide (VI), pale yellow, m. 270-1' (PhNO2). Through a suspension of 4.3 g. III in 60 ml. anhydrous CCl4 containing n.

0.2 g.
iodine, anhydrous Cl was bubbled to complete dissoln., excess Cl removed

bubbling dry air, the solution, containing 4,2-O2N(C1S)C6H3COC1 (VII),

added dropwise, with stirring and cooling, to 12 ml. 20% aqueous NH3, the mixture kept 2 hrs. at room temperature, the precipitate filtered off, washed with petr. ether, and suspended in a little H2O, the mixture acidified with dilute HCl, and the precipitate filtered off and washed with H2O to yield 6-nitro-1,2-benzoisothiazolone (VIII), yellow, m. 280° (EtOH) (decomposition). VII (from 4.3 g. III) in anhydrous CCl4 was added dropwise to a solution of 5 g. BuNH2 in 20 ml.

L10 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

94803-44-8 CAPLUS 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-3-phenyl-7a-(1-pyrrolidinyl)- (7CI, 9CI) (CA INDEX NAME)

95867-96-2 CAPLUS 2-Isoxazoline, 3.4,5-triphenyl-5-(1-pyrrolidinyl)- (7CI) (CA INDEX NAME)

97847-70-6 CAPLUS 4H-Cyclopent(d)isoxazole, 3a,5,6,6a-tetrahydro-3-phenyl-6a-(1-pyrrolidinyl)- (7CI, 9CI) (CA INDEX NAME)

98563-49-6 CAPLUS
4H-Cyclohept [dlisoxazole, 3a,5,6,7,8,8a-hexahydro-3-phenyl-8a-(1-pyrrolidinyl)- (TCI) (CA INDEX NAME)

L10 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued) anhyd. CC14, the mixt. kept 1 hr., filtered, and the filtrate evapd. in vacuo at 40° to yield 2-butyl-6-nitro-1,2-benzioschizazolone (IX), yellow, m. 109-10° (C6H6-ligroine). VII analogously treated with PhNIZ yielded 2-phenyl-6-nitro-1,2-benzioschizazolone (IX), yellow, m. 229-31° (PhMe). VIII (1 g.) suspended in 10 ml. AcOR, 3 ml. 30t M2O2 added, and the mixt. heated on a water bath 1 hr. at 100° and evapd. to dryness in vacuo at 40°, yielded 6-nitro-1,2-benzioschiarolone 1,1-dioxide m. 96-7° (70t EtOR), and X yielded 2-penyl-6-nitro-1,2-benziaschiarolone 1,1-dioxide, m. 96-7° (70t EtOR), and X yielded 2-penyl-6-nitro-1,2-benziaschiarolone 1,1-dioxide (XI), m. 183° (dil. EtOR). Dry pulverized VIII (2 g.) in 10 ml. AcOR was heated on a water bath 1 hr. at 100°, cooled, 5 vols. H20 added, and the ppt. filtered off and washed with H20 to yield 2-acetyl-6-nitro-1,2-benziaschiazolone, yellow, m. 220-2° (MeZCO). VIII (2 g.) treated in the same way with 10 ml. (EtCO)2CO, gave 2-propionyl-6-nitro-1,2-benziaschiazolone, yellow, m. 185-6° (CHC13). VIII in 100 alc. suspension was treated, with stirring and warming at 50° with an equimolar amt. 4N NaOH to give VIII Na salt, 2 g. of which was suspended in 30 ml. anhyd. C6H6, 1.3 g. BaCl added, the mixt. refluxed with stirring 1 hr., evapd. to dryness, and worked up to yield 2-benzyl-6-nitro-1,2-benzisothiazolone, yellow, m. 154-6° (PhMe). V. IX, and X inhibited the growth of Trichophyton mentagrophytes at a concn. of 0.5 y/ml. 7 references.

11 92647-93-3, 2-Isoxazoline, 4-ethyl-3-phenyl-5-(1-pyrrolidinyl)-93947-42-3, 1,2-Benzisoazole, 3a, 4,5,6,7,a-hexahydro-3-phenyl-73-(1-pyrrolidinyl)-93657-96-2 , 2-Isoxazoline, 3,4,5-triphenyl-5-(1-pyrrolidinyl)-9367-96-2 , 2-Isoxazoline, 3,4,5-triphenyl-5-(1-pyrrolidinyl)-97847-70-6, 4H-Cyclopent [d]:soxazole, 3a, 5,6,6-a-tetrahydro-3-phenyl-76-(1-pyrrolidinyl)-(preparation of)

RN 92647-93-3 CAPLUS

CN 2-Isoxazoline, 4-ethyl-3-phenyl-5-(1-pyrrolidinyl)-(7CI) (CA INDEX

93947-42-3 CAPLUS 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-7-methyl-3-phenyl-7a-(1-pyrrolidinyl)- (7CI) (CA INDEX NAME)

L10 ANSWER 59 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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L10 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2005 ACS ON STN ACCESSION NUMBER: 1964:82853 CAPLUS 60:82853 ORIGINAL REFERENCE NO.: 60:1450le-h
                                                                         1964:82853 CAPLAS
60:82853
60:14501e-h
Enamines. X. Reactions of halohydroxamic acids with
enamines of alicyclic compounds
Bianchetti, Gluseppe; Pocar, Donato; Dalla Croce,
  AUTHOR (S):
                                                                         Piero Univ. Milan Gazzetta Chimica Italiana (1963), 93(12), 1726-35 CODEN: GCITA9: ISSN: 0016-5603
  CORPORATE SOURCE:
SOURCE:
  CODEN: GCTTA9: ISSN: 0016-5603

LANGUAGE: Unavailable ,
OTHER SOURCE(S): CASREACT 60:82853

AB 1-(N-Morpholiny1)-1-cycloheptene, bl3 134*, was prepared by areotropic removal of H20 from equimolar amts. of cycloheptanone and morpholine in PhMe containing a trace of MeC6H4SO3H, followed by distillation
               illation
Similarly was prepared 1-(N-4-methylpiperazinyl)-1-cyclopentene, b0.15
116-18*. Equimolar amts. of II, 1-(N-morpholinyl)-1-cyclohexene,
and Et3N boiled in CHCl3 1 hr. and evaporated to an oil that solidified v
               V (R = 4-02NC6H4, n = 4, R' = N-morpholinyl), m. 138-40° (EtOH). Likewise, by boiling 45 min. to 1 hr. and using the resp. reagents were prepared the following derivs. of V: <math>(R = 4-02NC6H4, R' = N-morpholinyl),
```

which was extracted with Et20, filtered, evaporated, and the residue boiled 30

ed 30
min. with 100 cc. 10% NaOH and then acidified.
94803-44-8, 1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-3-phenyl-7a(1-pyrrolidinyl)(preparation of)
94803-44-8 CAPLUS
1,2-Benzisoxazole, 3a,4,5,6,7,7a-hexahydro-3-phenyl-7a-(1-pyrrolidinyl)(7CI, 9CI) (CA INDEX NAME)

L10 ANSWER 60 OF 60 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

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